

APPENDIX I-A

SUBSTANCES USED IN THE IRE TEST METHOD REANALYSIS

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Substances Used in the IRE Test Method Reanalysis

Substance	CASRN ⁷	Concentration Tested	Chemical Class	Product Class	pH	Form Tested	Purity	In Vivo Classification (GHS) ²³	Category I Subclass ⁴	In Vivo Classification (EPA) ^{3,6}	In Vivo Classification (EU) ^{7,8}	In Vitro Classification	Reference
Acetaldehyde	75-07-0	100%	ORGANIC	Flammable liquid used in manufacture of acetic acid, perfumes, and flavors		Solution					SCNM ⁹	Severe irritant	CEC (1991)
Acetic acid	64-19-7	10%	CARBOXYLIC ACID	Food preservative and acidifier; Solvent. Manufacture of acetates, acetyl compounds, cellulose acetate, rayon, plastics and rubber in tanning		Liquid					R41	Severe Irritant	CEC (1991)
Acetone	67-64-1	100%	KETONE	Solvent; Antiseptic; Chemical intermediate; Raw material		Liquid	99%	Category 2A		Category II	R36	Severe Irritant	Balls et al. (1995)
Acetone (F33)	67-64-1	100%	KETONE	Solvent; Antiseptic; Chemical intermediate; Raw material		Liquid	99%	Category 2A		Category II	R36	Severe Irritant	Guerriero et al. (2004)
2-(Acetoxy)-1-phenylethanone (F27)	-	100%	KETONE, ESTER	Raw material		Solid		Nonirritant		Category III	Nonirritant	Nonsevere Irritant	Guerriero et al. (2004)
Allyl alcohol (F34)	107-18-6	100%	ALCOHOL	Resins, Plasticizers, War gas, Allyl compounds		Liquid		NT ⁸		NT	NT	Severe Irritant	Guerriero et al. (2004)
gamma-(Aminocarbonyl)-N-methyl N,N-bis(1-methylethyl)-gamma-phenyl, iodide (F14)	-	100%	ONIUM, AMIDE	Active pharmaceutical ingredient		Solid		Category 2A		Category II	R36	Nonsevere Irritant	Guerriero et al. (2004)
1-(S-Amino-2-methoxyphenyl) piperazine hydrochloride (F20)	-	100%	HETEROCYCLE, AMINE	Chemical intermediate		Solid		Nonirritant		Category III	Nonirritant	Severe Irritant	Guerriero et al. (2004)
tetra-Aminopyrimidine sulfate	5392-28-9	100%	AMINE, HETEROCYCLE, SALT, INORGANIC	Developer		Solid	97%	Nonirritant		Category III	Nonirritant	Nonsevere Irritant	Balls et al. (1995)
Ammonium nitrate	6484-52-2	100%	SALT, INORGANIC, ONIUM	Fertilizer; Chemical intermediate; Industrial explosive		Solid	100%	Category 2B		Category III	R36	Nonsevere Irritant	Balls et al. (1995)
Ammonium nitrate (F36)	6484-52-2	100%	SALT, INORGANIC, ONIUM	Fertilizer; Chemical intermediate; Industrial explosive		Solid	>99.9%	Category 2B		Category III	R36	Nonsevere Irritant	Guerriero et al. (2004)
L-Aspartic acid	70-47-3	100%	AMINO ACID	Organic intermediate; Fungicides; Germicides		Solid	100%	SCNM ⁷		SCNM	SCNM	Nonsevere Irritant	Balls et al. (1995)
Benzalkonium chloride	8001-54-5	100%	INORGANIC SALT, ONIUM	Surfactant (cationic), Bactericide, Fungicide, Preservative		Solution					R41	Severe Irritant	CEC (1991)
Benzalkonium chloride (1 %)	8001-54-5	1%	ONIUM	Surfactant (cationic), Bactericide, Fungicide, Preservative		Solution	98%	Category I	1	Category I	R41	Severe Irritant	Balls et al. (1995)
Benzalkonium chloride (10%)	8001-54-5	10%	ONIUM	Surfactant (cationic), Bactericide, Fungicide, Preservative		Solution	98%	Category I	4	Category I	R41	Severe Irritant	Balls et al. (1995)
Benzalkonium chloride (5%)	8001-54-5	5%	ONIUM	Surfactant (cationic), Bactericide, Fungicide, Preservative		Solution	98%	Category I	3	Category I	R41	Severe Irritant	Balls et al. (1995)
3-((Benzylthio)methyl)-6-chloro-1,1-dioxide (F29)	-	100%	ETHER, SULFUR COMPOUND, ORGANIC	Active pharmaceutical ingredient		Solid		Nonirritant		Category IV	Nonirritant	Nonsevere Irritant	Guerriero et al. (2004)
Brij 35	9002-92-0	100%	ALCOHOL	Detergent, Solubilizer, Emulsifier, Lubricant		Solution					Nonirritant	Nonsevere Irritant	CEC (1991)
Butanol	71-36-3	100%	ALCOHOL	Solvent; Chemical intermediate; Flavor ingredient		Liquid					Nonirritant	Severe Irritant	CEC (1991)
iso-Butanol	78-83-1	100%	ALCOHOL	Solvent; Chemical intermediate; Flavor ingredient		Liquid	99.9%	Category 2A		Category II	R36	Severe Irritant	Balls et al. (1995)
n-Butanol (F35)	71-36-3	100%	ALCOHOL	Solvent; Chemical intermediate; Flavor ingredient		Liquid	99.9%	Category 2A		Category II	R36	Severe Irritant	Guerriero et al. (2004)
2-Butoxyethyl acetate	112-07-2	100%	ESTER	Solvent, Textile dyeing and printing, Leather treatment, Production of plasticizers, Stabilizer		Liquid					Nonirritant	Nonsevere Irritant	CEC (1991)

Substance	CASRN ¹	Concentration Tested	Chemical Class	Product Class	pH	Form Tested	Purity	In Vivo Classification (GHS) ^{2,3}	Category 1 Subclass ⁴	In Vivo Classification (EPA) ^{5,6}	In Vivo Classification (EU) ^{7,8}	In Vitro Classification	Reference
N-Butyl acetate	123-86-4	100%	ESTER	Solvent; Synthetic flavor ingredient		Liquid		Nonirritant		Category III	Nonirritant	Nonsevere Irritant	Balls et al. (1995)
n-Butyl acetate (F39)	123-86-4	100%	ESTER	Solvent; Synthetic flavor ingredient		Liquid	99%	Nonirritant		Category III	Nonirritant	Severe Irritant	Guerriero et al. (2004)
g-Butyrolactone	96-48-0	100%	HETEROCYCLE, LACTONE	Synthetic intermediate; Solvent		Liquid		Category 2A		Category II	R36	Severe Irritant	Balls et al. (1995)
Captan 90 concentrate	133-06-2	100%	IMIDE, SULFUR COMPOUND, ORGANIC	Pesticide		Solution	90%	Category I	4	Category I	R41	Nonsevere Irritant	Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	100%	CARBOXYLIC ACID, ALDEHYDE	Manufacturing impurity (polyester); Developer intermediate		Solid	>95%	Category 2A		Category II	R36	Nonsevere Irritant	Balls et al. (1995)
Cetylpyridium bromide (F37)	140-72-7	100%	ONIUM, HETEROCYCLE	Surfactant (cationic), Germicide, Laboratory reagent		Solid	98%	Category I	4	Category I	R41	Severe Irritant	Guerriero et al. (2004)
Cetylpyridinium bromide (0.1%)	140-72-7	0.1%	ONIUM, HETEROCYCLE	Surfactant (cationic), Germicide, Laboratory reagent		Solution	99%	Nonirritant		Category III	Nonirritant	Severe Irritant	Balls et al. (1995)
Cetylpyridinium bromide (10%)	140-72-7	10%	ONIUM, HETEROCYCLE	Surfactant (cationic), Germicide, Laboratory reagent		Solution	99%	Category I	4	Category I	R41	Severe Irritant	Balls et al. (1995)
Cetylpyridinium bromide (6%)	140-72-7	6%	ONIUM, HETEROCYCLE	Surfactant (cationic), Germicide, Laboratory reagent		Solution	99%	Category I	2	SCNM	R41	Severe Irritant	Balls et al. (1995)
5-Chloro-2,4-disulfamoyl chlorocetanilide (F22)	-	100%	AMIDE	Raw material		Solid		Nonirritant		Category IV	Nonirritant	Nonsevere Irritant	Guerriero et al. (2004)
Chloroform	67-66-3	100%	HYDROCARBON, HALOGENATED COMPOUND, ORGANIC	Solvent		Liquid				SCNM	Nonsevere irritant	CEC (1991)	
5-Chloro-3-methylbenzo[b]thiophene-2-sulfonyl chloride (F18)	-	100%	SULFUR COMPOUND, ORGANIC	Raw material		Solid		Nonirritant		Category III	Nonirritant	Nonsevere Irritant	Guerriero et al. (2004)
5-Chloro-N-[4-methoxy-3-(1-piperazinyl)phenyl]-3-methylbenzo[B]thiophene-2-sulfonamide monohydrochloride (F4)	-	100%	HETEROCYCLE, ETHER, AMIDE	Active pharmaceutical ingredient		Solid		Category I	4	Category I	R41	Severe Irritant	Guerriero et al. (2004)
Chlorhexidine	55-56-1	100%	AMIDINE	Disinfectant; Mouthwash; Anti-infective agent		Solid		Category I	4	SCNM	SCNM	Severe Irritant	Balls et al. (1995)
Cyclohexanol	108-93-0	100%	ALCOHOL	Solvent; Chemical intermediate		Liquid	97%	Category I	2	Category I	R41	Severe Irritant	Balls et al. (1995)
Dibenzoyl-L-tartaric acid	2743-38-6	100%	CARBOXYLIC ACID	Optical resolution agent		Solid		Category I	2	SCNM	R41	Nonsevere Irritant	Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	100%	ESTER, ORGANOPHOSPHOROUS COMPOUND	Not classified		Solid	99%	Category 2A		Category II	R36	Nonsevere Irritant	Balls et al. (1995)
Dibutyltin chloride	683-18-1	100%	ORGANOTIN COMPOUND	Molluscicide, Slime control in paper mills, Wood preservative, disinfectant, Biocide in cooling systems, Leather and textile processing		Solution					R41	Severe Irritant	CEC (1991)
3,4-Dichloroaniline hydrochloride (F11)	-	100%		Chemical intermediate		Solid		SCNM		SCNM	SCNM	Severe Irritant	Guerriero et al. (2004)
2,6-Dichlorobenzenesulfonyl chloride (F1)	6579-54-0	100%		Raw material		Solid		SCNM		SCNM	SCNM	Severe Irritant	Guerriero et al. (2004)
2,6-Dichlorobenzoyl chloride	4659-45-4	100%	ACYL HALIDE	Anti-infective; Anti-fungal; Preservative		Liquid	99%	Category 2A		Category II	SCNM	Nonsevere Irritant	Balls et al. (1995)
2,6-Dichloro-5-fluoro-beta-oxo-3-pyridinepropanoate (F16)	96568-04-6	100%	ESTER, KETONE, HETEROCYCLE	Chemical intermediate		Solid		Category 2B		Category III	Nonirritant	Nonsevere Irritant	Guerriero et al. (2004)
1-(3,4-Dichlorophenyl)-5-isopropylbiguanide HCl (F6)	537-21-3	100%	AMIDINE	Active pharmaceutical ingredient		Solid		Category I	NC	Category I	R41	Severe Irritant	Guerriero et al. (2004)
3,4-Dimethoxybenzaldehyde (F19)	120-14-9	100%	ALDEHYDE	Raw material		Solid		Nonirritant		Category III	Nonirritant	Nonsevere Irritant	Guerriero et al. (2004)
2,2-Dimethylbutanoic acid	595-37-9	100%	CARBOXYLIC ACID	Pharmaceutical metabolite		Liquid	96%	SCNM		Category I	SCNM	Severe Irritant	Balls et al. (1995)
Dimethyl carbonate (F30)	616-38-6	100%	CARBOXYLIC ACID	Raw material		Solid		Nonirritant		Category III	Nonirritant	Severe Irritant	Guerriero et al. (2004)

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2,5-Dimethylhexanediol	110-03-2	100%	ALCOHOL	Intermediate for pharmaceuticals, pesticides, perfumes		Solid	99.5%	Category 1	1	Category I	R41	Nonsevere Irritant	Balls et al. (1995)
Dimethyl sulfoxide	67-68-5	100%	SULFUR COMPOUND	Solvent; Antifreeze; Paint and varnish remover,		Solution					Nonirritant	Nonsevere Irritant	CEC (1991)
Ethanol	64-17-5	100%	ALCOHOL	Solvent; Beverages; Antifreeze agent		Liquid	100%	Category 2A		Category III	Nonirritant	Severe Irritant	Balls et al. (1995)
Ethyl acetate	141-78-6	100%	ESTER	Solvent; Synthetic flavoring		Liquid	99%	Nonirritant		Category III	Nonirritant	Severe Irritant	Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	100%	ALCOHOL	Solvent; Plasticizer		Liquid	99%	Category 2A		Category II	R36	Nonsevere Irritant	Balls et al. (1995)
Ethyl-2-methylacetacetate	609-14-3	100%	KETONE, ESTER	Not classified		Liquid	97%	Category 2B		Category III	Nonirritant	Severe Irritant	Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	100%	ESTER	Solvent		Liquid	99%	Nonirritant		Category III	Nonirritant	Nonsevere Irritant	Balls et al. (1995)
Fluorescein, sodium	518-47-8	100%	POLYCYCLIC COMPOUND, CYCLIC HYDROCARBON	Phthalic indicator dye; used to detect corneal lesions in ophthalmology		Solution					SCNM	Nonsevere irritant	CEC (1991)
p-Fluoraniline	371-40-4	100%	AMINE	Intermediate for herbicides; Dyes		Liquid	99%	SCNM		SCNM	SCNM	Severe Irritant	Balls et al. (1995)
Fomesafen, acid form (solid)	72128-02-0	100%	IMIDE, ETHER, NITRO COMPOUND	Pesticide		Solid	97.5%	Nonirritant		Category III	Nonirritant	Severe Irritant	Balls et al. (1995)
Glycerol	56-81-5	100%	ALCOHOL	Solvent; Plasticizer; Lubricant; Emollient; Drug vehicle		Liquid	>99.5%	Nonirritant		Category IV	Nonirritant	Nonsevere Irritant	Balls et al. (1995)
Glycerol	56-81-5	100%	ALCOHOL	Solvent; Plasticizer; Lubricant; Emollient; Drug vehicle		Solution					Nonirritant	Nonsevere Irritant	CEC (1991)
Glycerol (F41)	56-81-5	100%	ALCOHOL	Solvent; Plasticizer; Lubricant; Emollient; Drug vehicle		Liquid	>99%	Nonirritant		Category IV	Nonirritant	Nonsevere Irritant	Guerrero et al. (2004)
n-Hexane	110-54-3	100%	ACYCLIC HYDROCARBON	Solvent; Adhesive; Gasoline additive		Liquid					Nonirritant	Nonsevere Irritant	CEC (1991)
n-Hexanol	111-27-3	100%	ALCOHOL	Solvent; Chemical intermediate; Synthetic flavor ingredient		Liquid	98%	Category 2A		Category II	R36	Severe Irritant	Balls et al. (1995)
3-Hydroxy-2-phenyl-4-quinolinecarboxylic acid (F24)	485-89-2	100%	HETEROCYCLE, CARBOXYLIC ACID, ALCOHOL	Chemical intermediate		Solid		Nonirritant		Category II	Nonirritant	Nonsevere Irritant	Guerrero et al. (2004)
HZA-1	-	Undiluted	FORMULATION	Shampoos, Hair care		Solution		Category 1	1	Category I	R41	Severe irritant	Gettings et al. (1996)
HZB-1	-	25%	FORMULATION	Soaps and surfactants		Solution		Category 1	1	Category I	R41	Severe irritant	Gettings et al. (1996)
HZC-1	-	25%	FORMULATION	Shampoos, Hair care		Solution		Category 1	1	Category I	R41	Nonsevere irritant	Gettings et al. (1996)
HZD-1	-	25%	FORMULATION	Shampoos, Hair care		Solution		Category 2B		Category III	Nonirritant	Nonsevere irritant	Gettings et al. (1996)
HZE-1	-	Undiluted	FORMULATION	Soaps and surfactants		Solution		SCNM		Category I	SCNM	Nonsevere irritant	Gettings et al. (1996)
HZF-1	-	Undiluted	FORMULATION	Shampoos, Hair care		Solution		Category 1	1	Category I	R41	Nonsevere irritant	Gettings et al. (1996)
HZG-1	-	25%	FORMULATION	Shampoos, Hair care		Solution		Category 1	1	Category I	R41	Severe irritant	Gettings et al. (1996)
HZH-1	-	Undiluted	FORMULATION	Soaps and surfactants, cosmetics		Solution		Nonirritant		Category IV	Nonirritant	Nonsevere irritant	Gettings et al. (1996)
HZI-1	-	Undiluted	FORMULATION	Soaps and surfactants		Solution		Category 1	1	Category I	R41	Severe irritant	Gettings et al. (1996)
HZJ-1	-	Undiluted	FORMULATION	Shampoos, Hair care		Solution		Nonirritant		Category IV	Nonirritant	Nonsevere irritant	Gettings et al. (1996)
HZK-1	-	Undiluted	FORMULATION	Soaps and surfactants		Solution		Category 1	1	Category I	R41	Severe irritant	Gettings et al. (1996)
HZL-1	-	Undiluted	FORMULATION	Soaps and surfactants		Solution		Category 1	1	Category I	R41	Severe irritant	Gettings et al. (1996)
HZM-1	-	25%	FORMULATION	Shampoos, Hair care		Solution		Category 1	1	Category I	R41	Severe irritant	Gettings et al. (1996)
HZN-1	-	25%	FORMULATION	Shampoos, Hair care		Solution		Category 1	1	Category I	R41	Severe irritant	Gettings et al. (1996)
HZP-1	-	Undiluted	FORMULATION	Shampoos, Hair care		Solution		Nonirritant		Category III	Nonirritant	Severe irritant	Gettings et al. (1996)
HZQ-1	-	Undiluted	FORMULATION	Soaps and surfactants		Solution		Nonirritant		Category III	Nonirritant	Nonsevere irritant	Gettings et al. (1996)

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HZR-1	-	25%	FORMULATION	Soaps and surfactants		Solution		Category 1	1	Category I	R41	Nonsevere irritant	Gettings et al. (1996)
HZS-1	-	Undiluted	FORMULATION	Soaps and surfactants		Solution		Category 1	1	Category I	R41	Severe irritant	Gettings et al. (1996)
HZT-1	-	Undiluted	FORMULATION	Soaps and surfactants		Solution		Nonirritant		Category IV	Nonirritant	Nonsevere irritant	Gettings et al. (1996)
HZU-1	-	25%	FORMULATION	Soaps and surfactants		Solution		Category 2B		Category III	R36	Severe irritant	Gettings et al. (1996)
HZV-1	-	25%	FORMULATION	Shampoos, Hair care		Solution		Category 1	1	Category I	R41	Severe irritant	Gettings et al. (1996)
HZW-1	-	25%	FORMULATION	Soaps and surfactants		Solution		Category 1	1	Category I	R41	Nonsevere irritant	Gettings et al. (1996)
HZX-1	-	Undiluted	FORMULATION	Shampoos, Hair care		Solution		Category 1	1	Category I	R41	Nonsevere irritant	Gettings et al. (1996)
HZY-1	-	Undiluted	FORMULATION	Shampoos, Hair care		Solution		Category 1	1	Category I	R41	Nonsevere irritant	Gettings et al. (1996)
HZZ-1	-	Undiluted	FORMULATION	Soaps and surfactants		Solution		Nonirritant		Category IV	Nonirritant	Nonsevere irritant	Gettings et al. (1996)
Imidazole	288-32-4	100%	HETEROCYCLE	Anti-fungal; Enzyme inhibitor		Solid	99%	Category 1	4	Category I	R41	Severe Irritant	Balls et al. (1995)
1H-Indole-2,3-dione (F28)	91-56-5	100%		Raw material		Solid		Nonirritant		Category IV	Nonirritant	Nonsevere Irritant	Guerriero et al. (2004)
Iodine chloride with pyridine (1:1) (F10)	6443-90-9	100%		Raw material		Solid		Category 1	NC	Category I	R41	Severe Irritant	Guerriero et al. (2004)
di-Isopropyl aminoethyl diphenyl acetamide (F15)	-	100%	AMINE, AMIDE	Raw material		Solid		Category 2B		Category III	R36	Nonsevere Irritant	Guerriero et al. (2004)
Isopropyl dicyanamide (F9)	35695-36-4	100%	AMINE, NITRILE	Chemical intermediate		Solid		Category 1	NC	Category I	R41	Severe Irritant	Guerriero et al. (2004)
Maneb	12427-38-2	100%	AMINE, SALT, ORGANIC, UREA	Pesticide		Solid	90% (approx)	SCNM		Category III	SCNM	Severe Irritant	Balls et al. (1995)
Mebrophen hydramine HCl (F5)	13977-28-1	100%	ETHER, AMINE, SLAT	Active pharmaceutical ingredient		Solid		Category 1	NC	Category I	R41	Severe Irritant	Guerriero et al. (2004)
Mercuric chloride	7546-30-7	100%	INORGANIC	Topical antiseptic/disinfectant; corrosive agent		Solid		SCNM		SCNM	SCNM	Severe irritant	CEC (1991)
2-Methoxyethanol	109-86-4	100%	ALCOHOL	Solvent		Liquid					Nonirritant	Severe Irritant	CEC (1991)
1-(2-Methoxyphenyl)piperazine hydrogen sulfate (F2)	-	100%		Raw material		Solid		SCNM		SCNM	SCNM	Severe Irritant	Guerriero et al. (2004)
Methyl acetate	79-20-9	100%	ESTER	Solvent; Chemical intermediate; Synthetic flavor ingredient		Liquid	98%	Category 2A		Category II	R36	Severe Irritant	Balls et al. (1995)
6-(Methylamino)-2-pyridine ethanol formate (1:1) (salt) (F17)	-	100%	HETEROCYCLE, AMINE, CARBOXYLIC ACID, SALT	Chemical intermediate		Solid		Nonirritant		Category III	Nonirritant	Severe Irritant	Guerriero et al. (2004)
Methyl cyanoacetate	105-34-0	100%	ESTER, NITRILE	Adhesive; Pharmaceutical intermediate		Liquid	99%	Category 2A		Category II	R36	Nonsevere Irritant	Balls et al. (1995)
Methylcyclopentane	96-37-7	100%	HYDROCARBONS, CYCLIC	Solvent		Liquid	>99%	Nonirritant		Category III	Nonirritant	Nonsevere Irritant	Balls et al. (1995)
4,4'-Methylenebis-(2,6-di-tert-butylphenol) (F43)	118-82-3	100%	SULFUR COMPOUND, ORGANIC	Raw material		Solid		Nonirritant		Category III	Nonirritant	Nonsevere Irritant	Guerriero et al. (2004)
Methyl ethyl ketone	78-93-3	100%	KETONE	Solvent; Manufacture of lacquers, varnishes, cosmetics, pharmaceuticals		Liquid	99%	Category 2A		Category III	R36	Severe Irritant	Balls et al. (1995)
Methyl ethyl ketone (F38)	78-93-3	100%	KETONE	Solvent; Manufacture of lacquers, varnishes, cosmetics, pharmaceuticals		Liquid	99%	Nonirritant		Category III	Nonirritant	Severe Irritant	Guerriero et al. (2004)
Methyl isobutyl ketone	108-10-1	100%	KETONE	Solvent; Synthetic flavor; Drycleaning		Liquid	98%	Nonirritant		Category III	Nonirritant	Severe Irritant	Balls et al. (1995)
1-Naphthalene acetic acid	86-87-3	100%	CARBOXYLIC ACID, POLYCYCLIC COMPOUND	Pesticide		Solid	96%	Category 1	NC	Category I	SCNM	Nonsevere Irritant	Balls et al. (1995)

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1-Naphthalene acetic acid, Na salt	61-31-4	100%	SALT, ORGANIC, POLYCYCLIC COMPOUND, CARBOXYLIC ACID, SALT	Pesticide		Solid	95%	Category 1	1	Category I	R41	Severe Irritant	Balls et al. (1995)
2-Nitro-4-propoxyaniline (F23)	-	100%	NITRO COMPOUND, AMINE, ETHER	Chemical intermediate		Solid		Nonirritant		Category III	Nonirritant	Nonsevere Irritant	Guerriero et al. (2004)
2-Nitro-4-thiocyananiline (F7)	54029-45-7	100%	NITRO COMPOUND, AMINE, SULFUR COMPOUND, ORGANIC	Chemical intermediate		Solid		Category 1	NC	Category I	R41	Severe Irritant	Guerriero et al. (2004)
2-Nitro-4-thio-N-propylaniline (F21)	54393-89-4	100%	AMINE, NITRO COMPOUND, SULFUR COMPOUND, ORGANIC	Chemical intermediate		Solid		Nonirritant		Category III	Nonirritant	Severe Irritant	Guerriero et al. (2004)
n-Octanol	111-87-5	100%	ALCOHOL	Solvent; Fragrance		Liquid	>99%	Category 2A		Category II	R36	Severe Irritant	Balls et al. (1995)
tetra-N-Octylammonium bromide (F8)	14866-33-2	100%	ONIUM	Raw material		Solid		Category 1	NC	Category I	R41	Severe Irritant	Guerriero et al. (2004)
2-(4-Oxopentyl)-1H-isoindole-1,3 (2H)-dione (F26)	3197-25-9	100%	HETEROCYCLE	Chemical intermediate		Solid		Nonirritant		Category III	Nonirritant	Nonsevere Irritant	Guerriero et al. (2004)
(S)-1-Phenyl-N-propylamine (F13)	3789-59-1	100%		Raw material		Liquid		SCNM		SCNM	SCNM	Severe Irritant	Guerriero et al. (2004)
Polyethylene glycol 400	25322-68-3	100%	ALCOHOL, ETHER	Surfactant (nonionic), Lubricant, Plasticizer, Solvent		Liquid		Nonirritant		Category IV	Nonirritant	Severe Irritant	Balls et al. (1995)
Polyethylene glycol 400 (F44)	25322-68-3	100%	ALCOHOL, ETHER	Surfactant (nonionic), Lubricant, Plasticizer, Solvent		Liquid		Nonirritant		Category IV	Nonirritant	Nonsevere Irritant	Guerriero et al. (2004)
Potassium cyanate	590-28-3	100%	SALT, INORGANIC	Herbicide; Pharmaceutical intermediate		Solid	97%	SCNM		SCNM	SCNM	Nonsevere Irritant	Balls et al. (1995)
Promethazine HCl	58-33-3	100%	AMINE, HETEROCYCLE, SULFUR COMPOUND, ORGANIC	Antihistamine; Anti-nausea drug		Solid	98%	Category 1	3	Category I	R41	Severe Irritant	Balls et al. (1995)
iso-Propanol	67-63-0	100%	ALCOHOL	Solvent; Aerosol formulations (ingredient)		Liquid	99.9%	Category 2A		Category III	SCNM	Severe Irritant	Balls et al. (1995)
Propylene glycol (F42)	57-55-6	100%	ALCOHOL	Antifreeze, Solvent, Emulsifier, Resins, Inhibitor of fermentation and mold growth		Liquid		Nonirritant		Category IV	Nonirritant	Nonsevere Irritant	Guerriero et al. (2004)
Pyridine	110-86-1	100%	HETEROCYCLE	Solvent; Intermediate for pharmaceuticals, dyes, pesticides		Liquid	99.9+%	Category 1	3	Category I	R41	Severe Irritant	Balls et al. (1995)
4,4'-Pyridylpiperidine (F12)	-	100%		Raw material		Solid		SCNM		SCNM	SCNM	Severe Irritant	Guerriero et al. (2004)
Quinacrine	69-05-6	100%	AMINE, HETEROCYCLE, POLYCYCLIC COMPOUND	Anti-infective (anti-helmintic)		Solid		Category 1	3	Category I	R41	Nonsevere Irritant	Balls et al. (1995)
Silver nitrate	7761-88-8	3% in water	INORGANIC	Germicide		Solution		SCNM		SCNM	SCNM	Nonsevere irritant	CEC (1991)
Sodium dicyanamide (F3)	-	100%	AMIDE	Raw material		Solid		Category 1	NC	Category I	R41	Severe Irritant	Guerriero et al. (2004)
Sodium dodecyl sulfate	151-21-3	100%	ORGANIC SALT, CARBOXYLIC ACID SALT	Anionic detergent, Emulsifier, Lubricant, Solubilizer		Solution					R41	Severe Irritant	CEC (1991)
Sodium hydroxide	1310-73-2	1% in water	INORGANIC, ALKALI	Acid neutralizer; caustic agent		Solution					SCNM	Severe irritant	CEC (1991)
Sodium hydroxide (1%)	1310-73-2	1%	ALKALI	Caustic agent		Solution	Reagent grade	Category 2B		Category III	R36	Severe Irritant	Balls et al. (1995)
Sodium hydroxide (10%)	1310-73-2	10%	ALKALI	Caustic agent		Solution	Reagent grade	Category 1	4	Category I	R41	Severe Irritant	Balls et al. (1995)
Sodium hydroxide (F31)	1310-73-2	10%	ALKALI	Caustic agent		Liquid	Reagent grade	Category 1	4	Category I	R41	Severe Irritant	Guerriero et al. (2004)

Substance	CASRN ¹	Concentration Tested	Chemical Class	Product Class	pH	Form Tested	Purity	In Vivo Classification (GHS) ^{2,3}	Category I Subclass ⁴	In Vivo Classification (EPA) ^{5,6}	In Vivo Classification (EU) ^{7,8}	In Vitro Classification	Reference
Sodium lauryl sulfate (15 %)	151-21-3	15%	SALT, ORGANIC, CARBOXYLIC ACID, SALT	Surfactant (anionic), Detergent		Solution	98%	Category I	NC	Category I	SCNM	Nonsevere Irritant	Balls et al. (1995)
Sodium lauryl sulfate (3 %)	151-21-3	3%	SALT, ORGANIC, CARBOXYLIC ACID, SALT	Surfactant (anionic), Detergent		Solution	98%	Nonirritant		Category III	Nonirritant	Nonsevere Irritant	Balls et al. (1995)
Sodium oxalate	62-76-0	100%	SALT, ORGANIC, CARBOXYLIC ACID, SALT	Textile finishing; Pyrotechnic; Industrial byproduct		Solid	>99%	Category I	4	Category I	R41	Nonsevere Irritant	Balls et al. (1995)
Sodium perborate tetrahydrate	10486-00-7	100%	SALT, INORGANIC, BORON CONTAINING COMPOUND	Household cleaner; Detergent		Solid	98.6%	Category I	4	Category I	R41	Nonsevere Irritant	Balls et al. (1995)
4,4'-Sulfonylbisbenzenamine (F25)	80-08-0	100%	SULFUR COMPOUND, ORGANIC	Active pharmaceutical ingredient		Solid		Nonirritant		Category IV	Nonirritant	Nonsevere Irritant	Guerriero et al. (2004)
Toluene	108-88-3	100%	CYCLIC HYDROCARBON	Solvent; Gasoline additive; Manufacture of benzene derivatives, medicines, dyes, perfumes		Liquid	99%	Nonirritant		Category III	Nonirritant	Severe Irritant	Balls et al. (1995)
Toluene	108-88-3	100%	CYCLIC HYDROCARBON	Solvent; Gasoline additive; Manufacture of benzene derivatives, medicines, dyes, perfumes		Liquid					Nonirritant	Nonsevere Irritant	CEC (1991)
Toluene (F40)	108-88-3	100%	CYCLIC HYDROCARBON	Solvent; Gasoline additive; Manufacture of benzene derivatives, medicines, dyes, perfumes		Liquid	99%	Nonirritant		Category III	Nonirritant	Nonsevere Irritant	Guerriero et al. (2004)
Triacetin	102-76-1	100%	ESTER	Solvent, Fixative		Solution					Nonirritant	Nonsevere Irritant	CEC (1991)
Tributyltin chloride	688-73-3	100%	ORGANOTIN COMPOUND	Molluscicide, Slime control in paper mills, Wood preservative, disinfectant, Bioicide in cooling systems, Leather and textile processing		Solution					R41	Severe Irritant	CEC (1991)
Trichloroacetic acid (3%)	76-03-9	3%	CARBOXYLIC ACID	Caustic agent; Fixative; Herbicide		Solution	Reagent grade	Nonirritant		Category III	Nonirritant	Nonsevere Irritant	Balls et al. (1995)
Trichloroacetic acid (30%)	76-03-9	30%	CARBOXYLIC ACID	Caustic agent; Fixative; Herbicide		Solution	Reagent grade	Category I	4	Category I	R41	Severe Irritant	Balls et al. (1995)
Trichloroacetic acid (F32)	76-03-9	30%	CARBOXYLIC ACID	Caustic agent; Fixative; Herbicide		Liquid	Reagent grade	Category I	4	Category I	R41	Severe Irritant	Guerriero et al. (2004)
Triethanolamine	102-71-6	100%	AMINE, ALCOHOL	Chemical intermediate; Cosmetic ingredient; Vulcanization accelerator		Solution					Nonirritant	Nonsevere Irritant	CEC (1991)
Triton X-100 (10 %)	9002-93-1	10%	ETHER	Surfactant (nonionic), Detergent, Emulsifier		Solution	98%	Category I	NC	Category II	R41	Severe Irritant	Balls et al. (1995)
Triton X-100 (5 %)	9002-93-1	5%	ETHER	Surfactant (nonionic), Detergent, Emulsifier		Solution	98%	Category 2A		Category III	R36	Severe Irritant	Balls et al. (1995)
Tween 20	9005-64-5	100%	ESTER, ETHER	Surfactant (nonionic), Detergent		Solution	98%	Nonirritant		Category III	Nonirritant	Nonsevere Irritant	Balls et al. (1995)

Substances in bold indicate those that were included in the "Expanded data set" analyses described in the text.

¹CASRN=Chemical Abstracts Service Registry Number.

²GHS=Globally Harmonized System (UN [2003]).

³Eye Irritant Category 1 = irreversible effects on the eye/serious damage to the eye; Category 2A = reversible effects on the eye/irritating to the eyes; Category 2B = reversible effects on the eye/mildly irritating to the eyes; Nonirritant = not an eye irritant

⁴NICEATM-defined subgroups assigned based on the lesions that drove classification of a GHS Category 1 substance. 1: based on lesions that are persistent; 2: based on lesions that are severe (not including corneal opacity score equal to 4); 3: based on lesions that are severe (not including corneal opacity score equal to 4) and persistent; 4: corneal opacity score equal to 4 at any time; NC: No subclassification could be made based on the data.

Substance	CASRN ¹	Concentration Tested	Chemical Class	Product Class	pH	Form Tested	Purity	<i>In Vivo</i> Classification (GHS) ^{2,3}	Category I Subclass ⁴	<i>In Vivo</i> Classification (EPA) ^{5,6}	<i>In Vivo</i> Classification (EU) ^{7,8}	<i>In Vitro</i> Classification	Reference
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¹EPA=U.S. Environmental Protection Agency (EPA [1996]).

²Toxicity Category I for the Primary Eye Irritation Study = Corrosive, or corneal involvement or irritation not reversible within 21 days; Category II = Corneal involvement or irritation clearing in 8-21 days; Category III = Corneal involvement or irritation clearing in 7 days or less; Category IV = Minimal effects clearing within 24 hr.

³EU=European Union (EU [2001]).

⁴Risk phrase R41 = risk of serious damage to the eyes; R36 = irritating to the eyes; nonirritant = not an eye irritant.

⁵SCNM=Study Criteria Not Met.

⁶NT=Not tested.

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